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Risö Report No. 146

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Danish Atomic Energy Commission

Research Establishment Risö

Screening Corrections in the Spin Zero Approximation

by B. Eman

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Screening Corrections in the Spin Zero Approximation

by

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The Danish Atomic Energy Commission
Research Establishment Risö
Physics Department

Abstract

Corrections for screening in beta decay are calculated from the solutions of the Klein-Gordon equations with Hulthén and Coulomb potentials. The parameters of the Hulthén potentials are obtained by fitting to the Hartree curves and the Fermi-Thomas-Dirac potentials respectively.

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Contents

Introduction

The Coulomb interaction between charged particles, created in weak processes, and the rest of the nucleus is modified by the charge distribution in the nucleus and by the presence of the atomic charge. These corrections, called finite-size and screening corrections respectively, have been analysed by different authors[1-6]. Finite-size corrections have been extensively calculated and tabulated[4,5]. There is some ambiguity in the estimate of screening corrections since the choice of the screened potential affects the result. This potential is usually written in the form

$$V = \frac{Z\alpha}{r}\,\phi(r) \quad . \tag{1}$$

For $\phi(r)$, Reitz[2] used the solution of the Fermi-Thomas-Dirac (FTD) equation and Bühring[6] the approximate analytical expressions[7] of Hartree curves. In both cases the numerical integration of Dirac's equations was performed. The screening correction factors (ratio between Fermi functions for screened and Coulomb potentials) calculated by Reitz and by Bühring differ considerably.

We have introduced the assumption that the effect of screening on the radial wave functions of electrons is spin independent, i.e. it is the same whether the particle has spin one half or zero. The calculation of screening correction factors may then be considerably simplified because, as such a factor, we use the ratio between Fermi functions obtained from solutions of the Klein-Gordon equations with Hulthén[8] and Coulomb potentials respectively.

We first describe the determination of the parameters of the Hulthen potentials and then make a comparison with the results of Bühring. The method of solving the Klein-Gordon equation is outlined in the appendix.

1. Choice of the Potential

The solutions of the Klein-Gordon equation with zero angular momentum for the Hulthén potential

$$V_H = Z \cdot \alpha \cdot \frac{\lambda\, e^{-\lambda r}}{1 - e^{-\lambda r}} \tag{2}$$

are available (see appendix and ref. 8). The parameter λ in (2) has to be chosen in such a way that eq. (2) reproduces the actual atomic potentials. It is obvious that with the one-parameter function (2) we shall be unable to reproduce the actual atomic potentials in a wide region of radius r. It seems reasonable to confine oneself to the region of small r because we make use of the solutions of the Klein-Gordon equation at the nuclear radius.

As an actual atomic potential we may use the values obtained by the Hartree self-consistent field calculations[13,14]. The Herman-Skillman tables of atomic potentials[14] differ from others[13] by taking into account that the electron does not interact with itself. Normalization of eq. (2) to the tabulated potentials[14] was done at $x = 0.01$, where x is the radius in Thomas-Fermi units, $x = \mu r = 1.13 \cdot a \cdot Z^{1/3} \cdot r$. The results obtained are given in fig. 1. Instead of plotting the parameter λ versus Z, we have plotted D, where $\lambda = 2 \cdot D \cdot a \cdot Z^{1/3}$.

On the other hand, when we use the tables of effective charges from ref. 13 and perform a normalization at the lowest tabulated value of the radius, the values obtained for the parameter D range from 1.2 (for $Z = 8$) to 1.55 (for $Z = 92$). The average value of D for $20 < Z < 40$ is 1.45.

As already pointed out, it is not possible to reproduce the tabulated potentials with the one-parameter function (2) in the wide region of radius r. So, for the sake of comparison we also give the values of the parameter D obtained when the normalization points were taken at large distances. The range of D is in this case between 1.10 (for $Z = 8$) and 0.60 (for $Z = 92$).

Of course, in comparison with the Hartree method, the Thomas-Fermi-Dirac (TFD) statistical model cannot be considered better for describing the actual atomic potential, but for the sake of completeness we calculated the parameters D by means of the TFD functions[9]. At the nuclear radius D is 1.89 - 1.77, and for large distances, $0.4 \leqslant x \leqslant 1$, $D = 1.13$.

2. Results and Conclusion

The screening correction factors

$$S_{scr} = \frac{F_H(Z,E)}{F_c(Z,E)} , \tag{3}$$

where

$$F_H(Z,E) = (\lambda R)^{2\sigma-2} \left| \frac{\Gamma(\sigma+i\nu)\,\Gamma(\sigma+i\xi)}{\Gamma(2\sigma)\,\Gamma(1+2i\xi)} \right|^2 \left| F(\sigma+i\nu,\ \sigma+i\xi,\ 2\sigma,\ 1-e^{-\lambda R}) \right|^2 \tag{4}$$

and

$$F_c(Z,E) = (2pR)^{2\sigma-2} e^{\pi y} \left| \frac{\Gamma(\sigma+iy)}{\Gamma(2\sigma)} \right|^2 \left| {}_1F_1(\sigma+iy, 2\sigma, 2ipR) \right|^2 \quad (5)$$

(if $1-4\alpha^2 Z^2 > 0$; otherwise use equations (A 28) and (A 11)),

are calculated by using different values for the parameter D (tables 1 and 2), where $\lambda = 2 \cdot D \cdot \alpha \cdot Z^{1/3}$ and $R = 1.2\ A^{1/3} \cdot 10^{-13}$ cm. For other notations in eqs. (4) and (5) see the appendix. In calculating the screening correction factor (3), only the first two terms in the expansion of hypergeometric functions are taken into account. We stress that the advantage gained by this method in terms of simplicity is paid for by the ad hoc nature of the assumption that the effect of screening is independent of the spin.

The format of our table 1 has been selected so as to allow easy comparison with similar tables of Bühring. The range of the parameter D in table 1 was taken so as to cover the possible values of D according to different models of atomic potentials. This allows us to estimate the error in actual calculations of screening corrections. The most probable values of parameter D are given in fig. 1. The results presented in tables 1 and 2 indicate that the corrections for screening in beta decay are smaller than was believed according to the results of Reitz, which are incorporated in the tables of Dzelepov and Zyrianova[4].

The measurement of the capture to beta plus ratios in heavy elements would be a good experimental check of the screening corrections. If we take the Reitz values of the screening correction factors, the K/β^+ ratios in the 800 keV transition of ^{178}Ta and the 790 keV transition of ^{234}Np will be reduced by 14% and 17% respectively as compared with the values without any screening corrections. On the other hand, if we use our screening correction factors, these reductions will be only 6% in accordance with the results of Bühring.

Acknowledgements

It is a pleasure to thank Professor O. Kofoed-Hansen for his encouragement, Professor P.G. Hansen for helpful discussions, Leif Hansson of the GIER computer group at Risö for his kind assistance in the calculations, and the Danish Atomic Energy Commission for their hospitality at the Research Establishment Risö.

Appendix

A. Klein-Gordon Equation with the Coulomb Potential

The radial part of the Klein-Gordon equation for zero angular momentum

$$\left\{ \frac{d^2}{dr^2} + p - 2V(r)E + V^2(r) \right\} g_c(r) = 0 \tag{A 1}$$

and the Coulomb potential

$$V(r) = -\frac{Z\alpha}{r} \tag{A 2}$$

is of the type

$$\left\{ \frac{d^2}{dr^2} + A + \frac{B}{r} + \frac{C}{r^2} \right\} G(r) = 0 . \tag{A 3}$$

The regular solution of equation (A 3) is[11]

$$G(r) = \frac{1}{2} \left| e^{i\frac{\pi}{2}k} \frac{\Gamma(1/2+m-k)}{\Gamma(2m+1)} \right| e^{-i\frac{\pi}{2}(m+1/2)} M_{k,m}(z) , \tag{A 4}$$

where

$$M_{k,m}(z) = z^{1/2+m} e^{-z/2} {}_1F_1(1/2+m-k,\ 2m+1,\ z) , \tag{A 5}$$

$$k = -i \frac{B}{2\sqrt{A}} , \quad m = \frac{1}{2}\sqrt{1-4C} , \quad z = 2i\sqrt{A} \cdot r$$

and ${}_1F_1(a, b, c)$ is a hypergeometric function.

According to (A 3), (A 4) and (A 5) the regular solution of equation (A 1) for the potential (A 2) is

$$g_c(r) = \frac{1}{2} e^{\frac{\pi y}{2}} \left| \frac{\Gamma(\sigma+iy)}{\Gamma(2\sigma)} \right| e^{-i\frac{\pi}{2}\sigma} (2ipr)^{\sigma} e^{-ipr} {}_1F_1(\sigma+iy, 2\sigma, 2ipr) , \tag{A 6}$$

where

$$y = \frac{Z\alpha E}{p} \quad \text{and} \quad \sigma = \frac{1}{2} + \frac{1}{2}\sqrt{1 - 4\alpha^2 Z^2} . \tag{A 7}$$

Because of the singularity of the function $g_c(r)$ the Fermi function $F_c(Z, E)$ has to be taken at the nuclear radius R:

$$F_c(Z,E) = \left| \frac{g_c(r)}{p \cdot r} \right|^2_{r=R} . \tag{A 8}$$

For the sake of convenience we will change the notation slightly, putting

$$\sigma = \frac{1}{2} + S \tag{A 9}$$

$$S = \frac{1}{2} \left| \sqrt{1 - 4\alpha^2 Z^2} \right| .$$

Then

$$F_c(Z,E) = (2pR)^{2S-1} \, e^{\pi y} \left| \frac{\Gamma(\frac{1}{2} + S + iy)}{\Gamma(2S+1)} \right|^2 \left| {}_1F_1(\tfrac{1}{2} + S + iy, 1+2S, 2ipR) \right|^2 \tag{A 10}$$

for $1 - 4\alpha^2 Z^2 > 0$

and

$$F_c(Z,E) = \frac{e^{\pi(y-S)}}{2pR} \left| \frac{\Gamma(\frac{1}{2} + i(S+y))}{\Gamma(1+2iS)} \right|^2 \left| {}_1F_1(\tfrac{1}{2} + i(S+y), 1+2iS, 2ipR) \right|^2 \tag{A 11}$$

for $1 - 4\alpha^2 Z^2 < 0$.

B. Klein-Gordon Equation with the Hulthen Potential

Inserting in the Klein-Gordon equation (A 1) the Hulthén potential

$$V(r) = -Z\alpha \frac{\lambda e^{-\lambda r}}{1-e^{-\lambda r}} , \tag{A 2'}$$

we obtain[8]

$$\left\{ \frac{d^2}{dr^2} + p^2 + \frac{b\, e^{-\lambda r}}{1-e^{-\lambda r}} + \frac{a\, e^{-2\lambda r}}{(1-e^{-\lambda r})^2} \right\} g_H(r) = 0 , \tag{A 12}$$

where

$$a = \alpha^2 \lambda^2 Z^2$$

$$b = 2\alpha\lambda Z E . \tag{A 13}$$

Inserting

$$g_H(r) = e^{-ipr} \phi(r) \tag{A 14}$$

and

$$t = e^{-\lambda r} \tag{A 15}$$

in eq. (A 2), we obtain

$$\left\{ \frac{d^2}{dt^2} + \frac{1+2i\frac{p}{\lambda}}{t} \frac{d}{dt} + \frac{b}{\lambda^2 t(1-t)} + \frac{a}{\lambda^2 (1-t)^2} \right\} \phi(t) = 0. \tag{A 16}$$

In the next step the following substitution is useful:

$$\phi(t) = (1-t)^{\sigma} \quad \theta(t) \quad , \tag{A 17}$$

where σ is given by eq. (A 7). By inserting (A 17) into (A 16) we obtain

$$\left\{ t(1-t) \frac{d^2}{dt^2} + \left[1+2i\frac{p}{\lambda} - (2\sigma + 1 + 2i\frac{p}{\lambda})\, t \right] \frac{d}{dt} - \right.$$

$$\left. - \left[\sigma(1 + 2i\frac{p}{\lambda}) - \frac{b}{\lambda^2} \right] \right\} \theta(t) = 0 \quad . \tag{A 18}$$

In this way equation (A 12) is reduced to the hypergeometric equation

$$z(1-z) \frac{d^2u}{dz^2} + \left[c - (a+b+1)z \right] \frac{du}{dz} - abu = 0 \quad . \tag{A 19}$$

Of 24 solutions of (A 19) (ref. 12, sections 14.3 and 14.4) we are interested in those with the boundary conditions $g_H(o) = 0$ and $\lim_{r \to \infty} g_H(r) = \sin(pr + \Phi)$. The solution

$$u_{17} = F(a, b, 1 - c + a + b, 1-z) \tag{A 20}$$

satisfies these requirements.

From (A 20), (A 19), (A 18), (A 17), (A 16), (A 15), and (A 14) the non-normalized solution with the proper boundary conditions is

$$g_H(r) = N\, e^{-ipr} (1-e^{-\lambda r}) \quad F(\sigma+i\nu,\ \sigma+i\xi,\ 2\sigma,\ 1-e^{-\lambda r}) \quad , \tag{A 21}$$

where

$$\nu = \frac{1}{\lambda} (p + \sqrt{p^2 + a - b}) \tag{A 22}$$

$$\xi = \frac{1}{\lambda} (p - \sqrt{p^2 + a - b}) \quad . \tag{A 23}$$

The normalization factor N can be determined by means of the relation between hypergeometric functions with z and 1-z (ref. 12, section 14.53)

$$\lim_{r\to\infty} e^{-ipr} F(\sigma+iv,\ \sigma+i\xi,\ 2\sigma,\ 1-e^{-\lambda r}) =$$

$$\lim_{r\to\infty} \left\{ \frac{\Gamma(1+2i\frac{p}{\lambda})\,\Gamma(2\sigma)}{2i\frac{p}{\lambda}\,\Gamma(\sigma+iv)\,\Gamma(\sigma+i\xi)}\, e^{ipr}\, F(\sigma-iv,\ \sigma-i\xi,\right.$$

$$1-2i\frac{p}{\lambda},\ e^{-\lambda r}) - \frac{\Gamma(1-2i\frac{p}{\lambda})\ \Gamma(2\sigma)}{2i\frac{p}{\lambda}\,\Gamma(\sigma-iv)\ \Gamma(\sigma-i\xi)}\, e^{-ipr} \quad x$$

$$\left. F(\sigma+iv,\ \sigma+i\xi,\ 1+2i\frac{p}{\lambda},\ e^{-\lambda r}) \right\} =$$

$$\frac{\lambda}{p} \left| \frac{\Gamma(1+2i\frac{p}{\lambda})\ \ \Gamma(2\sigma)}{\Gamma(\sigma+iv)\ \ \Gamma(\sigma+i\xi)} \right| \quad \sin(pr + \Phi_o), \qquad \text{(A 24)}$$

where

$$\Phi_o = \arg \left| \frac{\Gamma(2\sigma)\ \ \Gamma(1+2i\frac{p}{\lambda})}{\Gamma(\sigma+iv)\ \Gamma(\sigma+i\xi)} \right| .$$

From (A 24) we obtain for the normalization factor N

$$N = \frac{p}{\lambda} \left| \frac{\Gamma(\sigma+iv)\ \ \Gamma(\sigma+i\xi)}{\Gamma(2\sigma)\ \ \ \Gamma(1+2i\frac{p}{\lambda})} \right| . \qquad \text{(A 25)}$$

Again the Fermi function has to be determined at the nuclear radius R:

$$F_H(Z,E) = \left| \frac{g_H(r)}{pr} \right|^2_{r=R} . \qquad \text{(A 26)}$$

Using (A 25), (A 21) and (A 9), we have

$$F_H(Z,E) = (\lambda R)^{2S-1} \left| \frac{\Gamma(\frac{1}{2}+S+i\nu) \quad \Gamma(\frac{1}{2}+S+i\xi)}{\Gamma(1+2S) \quad \Gamma(1+2i\frac{p}{\lambda})} \right|^2 \quad x$$

$$\left| F(\tfrac{1}{2}+S+i\nu\ ,\ \tfrac{1}{2}+S+i\xi\ ,\ 1+2S,\ 1-e^{-\lambda R}) \right|^2 \tag{A 27}$$

for $1 - 4\,\alpha^2 Z^2 > 0$

and

$$F_H(Z,E) = \frac{(1-e^{-\lambda R})}{\lambda^2 R^2} \left| \frac{\Gamma(\frac{1}{2}+i(S+\nu)) \quad \Gamma(\frac{1}{2}+i(S+\xi))}{\Gamma(1+2iS) \quad \Gamma(1+2i\frac{p}{\lambda})} \right| \quad x$$

$$\left| F(\tfrac{1}{2}+i(S+\nu),\ \tfrac{1}{2}+i(S+\xi),\ 1+2iS,\ 1-e^{-\lambda R}) \right|^2 \tag{A 28}$$

for $1 - 4\,\alpha^2 Z^2 < 0$.

We can also prove that our solutions $F_H(Z,E)$ approach $F_c(Z,E)$ when $\lambda \to 0$. From the definition of the hypergeometric functions it follows immediately that

$$\lim_{\lambda \to 0} F(\sigma+i\nu,\ \sigma+i\xi,\ 2\sigma,\ 1-e^{-\lambda R}) = {}_1F_1(\sigma+iy,\ 2\sigma,\ 2ipR)\ . \tag{A 29}$$

For $|\Gamma(z)|^2$ the next approximation is valid; if $x \approx 1$ and $y \gg 1$, we have

$$|\Gamma(x+iy)|^2 \approx 2\pi\ y^{2x-1}\ e^{-\pi y}\ . \tag{A 30}$$

By way of example we shall calculate the limits of eq. (A 27). Using (A 29) and (A 30), we have

$$\lim_{\lambda \to 0} F_H(Z,E) = \lim_{\lambda \to 0} \left\{ (\lambda R)^{2S-1} \quad \frac{\nu^{2S}\, e^{-\pi\nu}}{\frac{2p}{\lambda}\ e^{-\pi 2\frac{p}{\lambda}}} \left| \frac{\Gamma(\frac{1}{2}+S+i\xi)}{\Gamma(2S+1)} \right|^2 \quad x \right.$$

$$\left. \left| F(\tfrac{1}{2}+S+i\nu\ ,\ \tfrac{1}{2}+S+i\xi\ ,\ 2S+1,\ 1-e^{-\lambda R}) \right|^2 \right\} .$$

As for $\lambda \to o$

$$\nu \to \frac{2p}{\lambda} - \frac{Z\alpha E}{p}$$

$$\xi \to \frac{Z\alpha E}{p} = y\ ,$$

we have

$$\lim_{\lambda \to o} F_H(Z, E) = (2pR)^{2S-1}\ e^{\pi y}\ \left| \frac{\Gamma(\frac{1}{2} + S + iy)}{\Gamma\ (2S + 1)} \right|^2 \quad x$$

$$\left| {}_1F_1\ (\tfrac{1}{2} + S + iy,\ 2S + 1,\ 2ipR) \right|^2 = F_c(Z, E)\ ,$$

Q. E. D.

For positrons change Z to -Z in all expressions.

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Table 1

Screening correction factors S_{scr} *

Z(A)	17(35)			30(64)			50(114)			-7(14)				-26(54)				-56(136)			
p	D 1.45	0.76	B	D 1.45	0.70	B	D 1.45	0.66	B	D 1.45	1.13	1.03	B	D 1.45	1.13	0.66	B	D 1.45	1.13	0.66	B
0.2	0.9923	0.9959	0.9883	0.9963	0.9981	0.9911		0.9977	0.9751	1.0517	1.0404	1.0369	1.0449	2.6343	1.7655	1.4311	1.9[illegible]38	21.094	13.525	5.9485	16.870
0.4	0.9922	0.9959	0.9888	0.9929	0.9966	0.9892	0.9951	0.9978	0.9734	1.0101	1.0079	1.0072	1.0093	1.1181	1.0923	1.0523	1.1234	1.7396	1.5655	1.3204	1.7636
0.6	0.9945	0.9971	0.9913	0.9930	0.9966	0.9901	0.9944	0.9974	0.9759	1.0045	1.0035	1.0032	1.0043	1.0406	1.0317	1.0186	1.0[illegible]30	1.2033	1.1586	1.0927	1.2390
0.8	0.9960	0.9978	0.9934	0.9940	0.9971	0.9912	0.9942	0.9974	0.9776	1.0027	1.0021	1.0019	1.0027	1.0207	1.0162	1.0095	1.0[illegible]54	1.0889	1.0695	1.0408	1.1158
1.0	0.9970	0.9984	0.9941	0.9950	0.9976	0.9924	0.9945	0.9975	0.9795	1.0019	1.0015	1.0014	1.0020	1.0130	1.0101	1.0059	1.0[illegible]70	1.0489	1.0332	1.0225	1.0704
1.2	0.9976	0.9988	0.9953	0.9958	0.9980	0.9933	0.9950	0.9978	0.9815	1.0015	1.0012	1.0011	1.0016	1.0093	1.0072	1.0042	1.0123	1.0310	1.0243	1.0142	1.0488
1.4	0.9981	0.9990	0.9959	0.9964	0.9983	0.9940	0.9955	0.9980	0.9832	1.0013	1.0010	1.0009	1.0013	1.0072	1.0056	1.0033	1.0102	1.0217	1.0170	1.0099	1.0370
1.6	0.9984	0.9992	0.9961	0.9969	0.9985	0.9946	0.9960	0.9982	0.9848	1.0011	1.0009	1.0008	1.0011	1.0058	1.0046	1.0027	1.0088	1.0163	1.0127	1.0075	1.0297
1.8	0.9987	0.9994	0.9965	0.9973	0.9987	0.9953	0.9965	0.9984	0.9861	1.0010	1.0008		1.0010	1.0050	1.0039	1.0024	1.0075	1.0129	1.0101	1.0059	1.0249
2.0	0.9989	0.9995	0.9967	0.9977	0.9988	0.9956	0.9968	0.9986	0.9871	1.0009			1.0009	1.0043	1.0034	1.0021	1.0066	1.0107	1.0083	1.0049	1.0214

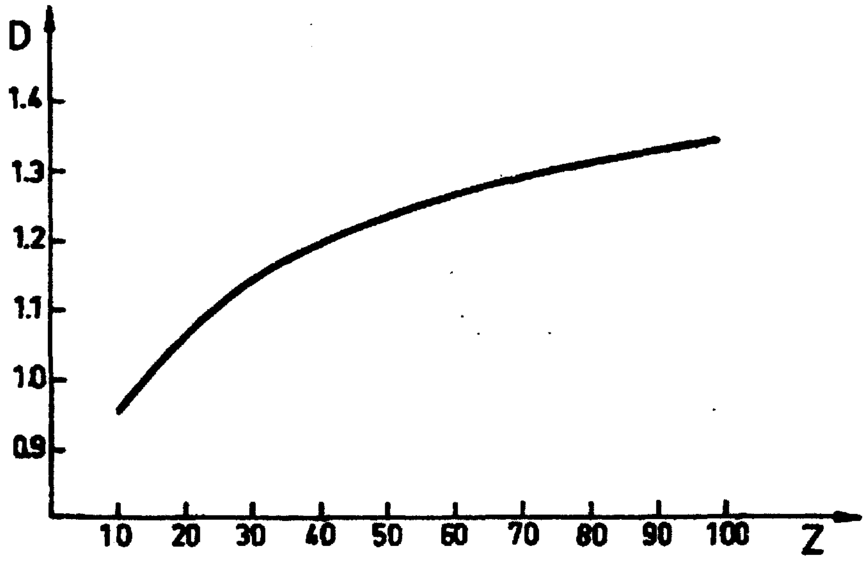
* Upper and lower values for the parameter *D* are obtained from Hartree potentials at small and large values of the radius, respectively. The value D = 1.13 corresponds to the TFD potentials[13] and to the Fermi-Thomas radius x = 0.4.

B Bühring's results[6].

Table 2

Screening correction factors obtained by using the values of the parameter D from fig. 1

Z(A) / p	-20(40)	-30(68)	-40(91)	-50(119)	-60(144)	-70(173)	-80(200)	-90(232)
0.2	1.3574	2.1577	4.1209	9.2725	23.802	68.747	221.84	746.94
0.4	1.0491	1.1275	1.2580	1.4617	1.7649	2.2101	2.8920	3.8732
0.6	1.0179	1.0424	1.0799	1.1339	1.2067	1.2992	1.4276	1.5863
0.8	1.0095	1.0210	1.0376	1.0602	1.0890	1.1220	1.1897	1.2264
1.0	1.0062	1.0129	1.0231	1.0339	1.0482	1.0621	1.0850	1.1119
1.2	1.0045	1.0091	1.0149	1.0220	1.0301	1.0362	1.0488	1.0636
1.4	1.0036	1.0069	1.0110	1.0157	1.0207	1.0231	1.0308	1.0398
1.6	1.0030	1.0054	1.0087	1.0121	1.0153	1.0158	1.0209	1.0267
1.8	1.0025	1.0047	1.0071	1.0097	1.0119	1.0115	1.0150	1.0190
2.0	1.0022	1.0041	1.0061	1.0081	1.0097	1.0087	1.0112	1.0141



Parameter D of the Hulthen potential as a function of the atomic charge Z.